Pairing in Asymmetrical Fermi Systems with Intra- and Inter-Species Correlations

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We consider inter- and intra-species pairing interactions in an asymmetrical Fermi system. Using equation of motion method, we obtain coupled mean-field equations for superfluid gap functions and population densities. We construct a phase diagram across BCS-BEC regimes. Inclusion of intra-species correlations result in stable polarized superfluid phase on BCS and BCS sides of unitarity at low polarizations. For larger polarizations, we find phase separations in BCS and BEC regimes. A superfluid phase exists for all polarizations deep in BEC regime. Our results should be apply broadly to ultra-cold fermions, nuclear and quark matter.

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Pairing in two-species Fermi systems with unequal population is of great current interest and importance across a wide range of fields and systems. Examples are unequal density mixtures of fermionic cold atoms [1, 2]; arbitrarily polarized liquid ^3He; superconductors in external magnetic field [3], in strong spin-exchange field [4, 5, 6], or with overlapping bands [7, 8]; isospin asymmetric nuclear matter [9] and dense quark matter exhibiting color superconductivity [10]. Unequal density cold fermions serve as prototypical systems, providing an unprecedented window into exploring superfluidity with tunable repulsive and attractive interactions. These are attained by sweeping across with s- or p-wave Feshbach resonances, thereby allowing the study of fermion ground states in both BCS and BEC regimes.

Among the *outstanding* questions in asymmetrical Fermi systems is the nature of the ground state in the BCS and BEC regimes, and whether the BCS superfluid state can sustain any finite imbalance between the species. Thus, it is important to arrive at a plausible phase diagram as a function of pairing interaction strength and species imbalance. Two-species systems are conveniently characterized as two pseudo-spin systems. It is believed that the BCS ground state in a finite magnetic field h, is robust against spin polarizations for $h \sim \Delta$, (Δ being the superconducting gap); beyond this it becomes unstable to a normal state. For *equal population* cold atom systems, there is theoretical agreement with experiments that find superfluid states in both BCS and BEC regimes with a "smooth crossover" around the "unitarity limit"(diverging singlet scattering length a_s).

For systems with *population imbalance*, various theoretical scenarios have been proposed [11, 12, 13]. Mean-field calculations [12, 13] find the superfluid state to be unstable to phase separation into superfluid and normal states or a mixed phase in the BCS regime; a superfluid state stabilizes however deep in the BEC regime. Currently there is intense experimental efforts in unequal density cold fermion atoms. One experiment [2] observed a transition from a polarized superfluid to phase separation at a polarization $\sim 10\%$ near unitarity on the BEC

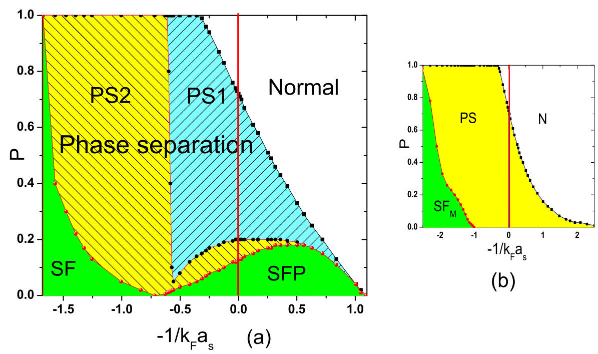

FIG. 1: (Color online) Polarization P vs s-wave coupling, $-1/(k_F a_s)$ phase diagram for asymmetrical fermions:(a) with a representative intra-species correlation strength $g_1 = 20$, corresponding to $1/(k_F^3 a_t) = 1.25$; (b) without intra-species correlations, $g_1 = 0$ (also obtained in Ref [13]). Vertical line refers to the unitarity limit; PS1, PS2, PS to phase separated regions; N to normal state.

side. To date, theoretical calculations have mostly considered *inter-species* s-wave interaction, and have ignored *intra-species* correlations. Ho et al [14] attempted to incorporate triplet correlations in a somewhat phenomenological manner; Huang et al [15] recently explored the implications for a FFLO state; Monte Carlo calculations [16] hint at a polarized superfluid phase near unitarity.

In this paper, we address the issue of the nature of the zero temperature (T=0) ground state of an asymmetrical Fermi system for arbitrary repulsive/attractive interaction strength and polarization. We also examine if the BCS superfluid state can sustain a finite population imbalance. While the unequal density cold fermion systems may provide a way to test our results, our paper should have a broader appeal, viz. electronic superconductivity, nuclear and quark matter superfluidity, etc. Generally, both inter-species and intra-species correlations may be present in an asymmetrical Fermi system. These may

arise from the underlying fermionic potentials (atomic, electronic, nucleon-nucleon, quark-quark) or from effects of the medium, i.e. "induced" interactions [17, 18]. We include the simplest ones allowed by symmetry: s-wave contact interaction between the species, and a p-wave interaction within the species. Following Leggett [19] and Eagles [20], our discussion is in terms of BCS-type pairing in both the BCS and BEC regimes, with the chemical potentials for the two species determined self-consistently with the pairing gaps. We do a detailed *stability analysis* of the multitude of states obtained from our equations.

Our findings are *dramatically different* from those without intra-species correlations, Our proposed phase diagram, Fig. 1a, shows that at T=0, for smaller polarizations, and sufficiently large *intra-species* correlations, gapped polarized superfluidity (hereafter referred to as SFP) becomes *stable* on both BCS and BEC sides of the "unitarity" limit. Depending on the *inter-species* interaction strength, at some polarization, SFP becomes unstable via a 1st-order transition to *phase separation*, denoted by PS1. PS1 is characterized by a negative "susceptibility", $\delta P/\delta h$; P being the spin-polarization, and h the difference of the chemical potentials, playing the role of a "magnetic field". For a given *intra-species* interaction, and for sufficiently weak inter-species interaction, SFP and PS1 undergo transitions to the normal state on the BCS side. The gapped SFP persists into the BEC regime, sustaining progressively smaller polarizations. Deeper in the BEC regime, we find a superfluid phase (SF) at all polarizations. In the BEC regime, in addition to PS1, we find the existence of a somewhat different phase separated state, PS2, characterized by positive "susceptibility", but not satisfying requisite superfluid ground state stability criteria.

For our detailed study, we consider a two-species Fermi system with unequal "pseudo-spin" populations. To allow for both *inter-species* and *intra-species* correlations, and noting that pseudo-spin rotation invariance would be broken by unequal chemical potentials, we adopt a pairing Hamiltonian given by

$$
\begin{aligned}
H &= \sum_{k\sigma} \xi_{k\sigma} c^{+}_{k\sigma} c_{k\sigma} \\
&+ \sum_{kk'q\sigma} \frac{g^{\sigma\sigma}_{kk'}}{V} c^{+}_{k+q/2\sigma} c^{+}_{-k+q/2\sigma} c_{-k'+q/2\sigma} c_{k'+q/2\sigma} \\
&+ \sum_{kk'q} \frac{g^{\uparrow\downarrow}_{kk'}}{V} c^{+}_{k+q/2\uparrow} c^{+}_{-k+q/2\downarrow} c_{-k'+q/2\downarrow} c_{k'+q/2\uparrow} \qquad (1)
\end{aligned}
$$

where the pseudospin $\sigma =\uparrow,\downarrow$ denote for example the two hyperfine states of ultracold Fermi atoms. $c^{+}_{k\sigma}$ is the fermion creation operator with kinetic energy $\xi_{k\sigma} = \epsilon_{k\sigma} - \mu_\sigma$; μ_σ is the chemical potential of each of the species. $g^{\uparrow\uparrow}_{kk'}$, and $g^{\downarrow\downarrow}_{kk'}$ are the interactions between the up and down spins respectively, and V is the volume. The singlet interaction, $g^{\uparrow\downarrow}_{kk'}$ is taken to be a constant, g_o. This is usually expressed in terms of s-wave scattering length a_s using $(4\pi\hbar^2 a_s/m)^{-1} = g_o^{-1} + \sum_k (2\epsilon_k)^{-1}$. A mean-field decoupling is attained by introducing three order parameters or gap functions ($\sigma, \sigma' =\uparrow,\downarrow$) given by, $\Delta_{\sigma\sigma'}(k,q) = -\sum_{k'} g^{\sigma\sigma'}_{kk'} < c_{-k'+q/2\sigma} c_{k'+q/2\sigma'} >$ This results in a mean-field Hamiltonian given by:

$$
\begin{aligned}
H^{MF} &= \sum_{k\sigma} \xi_{k\sigma} c^{+}_{k\sigma} c_{k\sigma} - \sum_{k,\sigma} \Delta_{\sigma\sigma}(k,q) c^{+}_{k+q/2\sigma} c^{+}_{-k+q/2\sigma} - \sum_{k,\sigma} \Delta^{*}_{\sigma\sigma}(k,q) c_{-k+q/2\sigma} c_{k+q/2\sigma} - \sum_{k.\sigma} |\Delta_{\sigma\sigma}(k,q)|^2 / g^{\sigma\sigma}_{kk} \\
&- \sum_{k} \Delta_{\downarrow\uparrow}(k,q) c^{+}_{k+q/2\uparrow} c^{+}_{-k+q/2\downarrow} - \sum_{k} \Delta^{*}_{\downarrow\uparrow}(k,q) c_{-k+q/2\downarrow} c_{k+q/2\uparrow} - \sum_{k} |\Delta_{\downarrow\uparrow}(k,q)|^2 / g^{\downarrow\uparrow}_{kk} \qquad (2)
\end{aligned}
$$

We employ the *equation of motion* method using imaginary time normal and anomalous Matsubara Green's functions, $G_{\sigma\sigma'}(k,\tau)$, $F_{\sigma\sigma'}(k,\tau)$, respectively, and our mean-field Hamiltonian, H^{MF}. The coupled equations in terms of $\Delta_{\sigma\sigma'}$ are given by $G_{\sigma\sigma'}(k,\tau)$ and $F_{\sigma\sigma'}(k,\tau)$:

$$
\begin{aligned}
\partial_\tau G_{\sigma\sigma'}(k,\tau) &= -\delta(\tau)\delta_{\sigma\sigma'} - \xi_{k+q/2\sigma} G_{\sigma\sigma'}(k,\tau) \\
&+ \sum_{\sigma''} \Delta_{\sigma''\sigma}(k,q) F_{\sigma''\sigma'}(k,\tau) \qquad (3) \\
\partial_\tau F_{\sigma\sigma'}(k,\tau) &= \xi_{-k+q/2\sigma} F_{\sigma\sigma}(k,\tau) \\
&+ \sum_{\sigma''} \Delta^{*}_{\sigma\sigma''}(k,q) G_{\sigma''\sigma'}(k,\tau) \qquad (4)
\end{aligned}
$$

where τ is the imaginary time variable. These equations may be Fourier transformed in the usual way with $\tau \to iw_n$, $\partial_\tau \to -iw_n$, where $iw_n = (2n+1)\pi/\beta$ are the Matsubara frequencies, n being an integer and $\beta = 1/k_B T$.

Here we focus on a superfluid condensate of pairs with *zero center-of-mass momentum*, q. Thus, we do not consider the $q \neq 0$ Fulde-Ferrel-Larkin-Ovchinnikov(FFLO) state [4, 5], but which may also be studied within this scheme. Solving the Fourier transformed equations at $q = 0$, we obtain the *2-point correlation functions*:

$$
G_{\sigma\sigma'}(k, iw_n) = \frac{\delta_{\sigma\sigma'} f_\sigma + \delta_{\sigma-\sigma'}(\Delta\Delta_\uparrow b_\downarrow - \Delta\Delta_\downarrow \Delta_\uparrow)}{D}
$$

$$F_{\sigma\sigma'}(k, iw_n) \;=\; \frac{\delta_{\sigma\sigma'} f_{\sigma\sigma} + \delta_{\sigma-\sigma'} f_{\sigma-\sigma}}{D} \tag{5}$$

where $f_\sigma = \Delta^2 b_{-\sigma} + \Delta^2_{-\sigma} b_\sigma - a_{-\sigma} b_\sigma b_{-\sigma}$; $f_{\sigma\sigma} = \Delta^2 \Delta_{-\sigma} + \Delta_\sigma \Delta^2_{-\sigma} - \Delta_\sigma a_{-\sigma} b_{-\sigma}$; $f_{\sigma-\sigma} = \Delta(\Delta^2 + \Delta_\sigma \Delta_{-\sigma} - a_\sigma b_{-\sigma})(\delta_{\sigma\downarrow} - \delta_{\sigma\uparrow})$; $D = (\Delta^2 + \Delta_\uparrow \Delta_\downarrow)^2 + a_\uparrow a_\downarrow b_\uparrow b_\downarrow - \sum_\sigma (\Delta^2 a_\sigma + \Delta^2_\sigma a_{-\sigma}) b_{-\sigma}$; with $a_\sigma = \xi_{k+q/2\sigma} - iw_n$, $b_\sigma = -\xi_{-k+q/2\sigma} - iw_n$. We have set $\Delta_{\uparrow\uparrow} \equiv \Delta_\uparrow$; $\Delta_{\downarrow\downarrow} \equiv \Delta_\downarrow$; $\Delta_{\uparrow\downarrow} \equiv \Delta$. The *excitation spectrum* can be found by examining the poles of the Green's functions, yielding the quasiparticle energies,

$$E^2_{k\pm} = (iw_n)^2 = (\alpha \pm \sqrt{\beta})/2 \tag{6}$$

where $\alpha = \xi^2_{k\uparrow} + \xi^2_{k\downarrow} + 2\Delta^2 + \Delta^2_1 + \Delta^2_2$, and $\beta = \left[(\xi^2_{k\uparrow} - \xi^2_{k\downarrow}) + (\Delta^2_1 - \Delta^2_2)\right]^2 + 4\Delta^2 \left[(\xi_{k\uparrow} - \xi_{k\downarrow})^2 + (\Delta_1 - \Delta_2)^2\right]$. Various quantities can now be obtained from our 2-point correlation functions. Thus, particle concentrations, n_σ for the two species ($\sigma = \uparrow, \downarrow$) are given by

$$\begin{aligned} n_\sigma &= \sum_k \left\langle c^+_{k\sigma} c_{k\sigma} \right\rangle = \sum_k \sum_{iw_n} \frac{1}{\beta} G_{\sigma\sigma}(k, iw_n) e^{iw_n 0^+} \\ &= \sum_k \sum_{l=\pm} (-1)^\lambda \left[\frac{n_F(E_{kl}) f_\sigma(k, E_{kl}) - n_F(-E_{kl}) f_\sigma(k, -E_{kl})}{2E_{kl}(E^2_{k+} - E^2_{k-})} \right] \end{aligned} \tag{7}$$

where λ is even for $l = +$, and odd for $l = -$; $n_F(E_{kl})$ are the Fermi functions. Likewise the three gaps equations are given by ($\sigma, \sigma' = \uparrow, \downarrow$):

$$\Delta_{\sigma\sigma'} = -\sum_k g^{\sigma\sigma'}_{kk} \sum_{iw_n} \frac{1}{\beta} F^*_{\sigma\sigma'}(k, iw_n) e^{iw_n 0^+} = -\sum_k \sum_{l=\pm} (-1)^\lambda g^{\sigma\sigma'}_{kk} \left[\frac{n_F(E_{kl}) f_{\sigma\sigma'}(k, E_{kl}) - n_F(-E_{kl}) f_{\sigma\sigma'}(k, -E_{kl})}{2E_{kl}(E^2_{k+} - E^2_{k-})} \right] \tag{8}$$

The above five equations are *coupled*, and can be solved self-consistently for the three gap functions, $\Delta, \Delta_\uparrow, \Delta_\downarrow$ for either fixed particle concentrations, $n_\uparrow$, $n_\downarrow$, or fixed chemical potentials, $\mu_\uparrow$, $\mu_\downarrow$.

We assume *equal masses* for the two species, and take the particle spectrum to be $\epsilon_k = \hbar^2 k^2/2m$. We adopt standard definitions: polarization, $P = (n_1 - n_2)/(n_1 + n_2)$; mean chemical potential $\mu = (\mu_1 + \mu_2)/2$; chemical potential difference $h = (\mu_1 - \mu_2)/2$; Fermi momentum $k_{F\sigma} = (6\pi^2 n_\sigma)^{1/3}$. Since $\sum_k f(k) \to \int_0^\infty f(k) \frac{d^3k}{(2\pi)^3} \to \int_0^\infty k^3_F f(k/k_F) \frac{d^3(k/k_F)}{(2\pi)^3}$, we can scale quantities having dimension of energy to ϵ_F. The *inter-species* interaction g_o is expressed in terms of coupling constant $\eta = -1/(k_F a_s)$. For the *intra-species* triplet interaction, we take the separable form $g^{\sigma\sigma}_{kk'} = g_1 \omega(k)\omega(k') Y_{10}(\hat{k}) Y_{10}(\hat{k'})$, where we have taken $g_{\uparrow\uparrow} = g_{\downarrow\downarrow} \equiv \tilde{g}_1$. More generally the $m = \pm 1$ terms would also be present; however this choice allows us to explore the consequences of intra-species correlations while keeping the calculations tractable. As a check, we also consider different types of momentum dependence: (i) $\omega(k) \propto$ *const*; (ii) $\omega(k) \propto k_0 k/(k^2_0 + k^2)$, a generalization of the Nozieres and Schmitt-Rink scheme [21]; (iii) $\omega(k) \propto \exp\left[-(k/k_0)^2\right]$, a Gaussian interaction; k_o being a cut-off momentum; these give qualitatively similar behavior. The first two forms of interaction require regularization due to ultraviolet divergence, while the third does not. With regularization, g_1 can be expressed in terms of a triplet scattering volume a_t [22]: $(4\pi\hbar^2 k^2_o a_t/m)^{-1} = g^{-1}_1 + \sum_k w(k)^2/(2\epsilon_k)$. Thus, $(3n/2\epsilon_F)\tilde{g}_1 \equiv g_1$ in our plots can be easily expressed in terms of a_t; e.g. $g_1 = 20$ corresponds to $1/(k^3_F a_t) = 1.25$.

For arbitrary inter-species s-wave and and intra-species p-wave pairing interactions, and population imbalances, we obtain self-consistent solutions of the $T = 0$ gap functions, $\Delta, \Delta_\uparrow, \Delta\downarrow$, and chemical potentials, μ_σ. On the BCS side, for a given g_o, the $\uparrow\downarrow$ gap Δ *decreases* with increasing intra-species interaction strength g_1, while at the same time both $\Delta_\uparrow, \Delta_\downarrow$ ($\Delta_\uparrow \neq \Delta_\downarrow$) increases, crossing at some value of g_1. The suppression of Δ is more pronounced at larger polarizations.

A proper construction of the asymmetrical Fermi system *phase diagram* requires a determination of stable ground states out of the manifold of paired condensates given by our equations [13, 23]. Accordingly, we carefully consider the stability criteria. The mean-field *ground state energy* as a function of the gaps at different polarizations, P is given by:

$$\begin{aligned} E_G \;\; &(\Delta, \Delta_\uparrow . \Delta_\downarrow) = \left\langle \Psi | H^{MF} | \Psi \right\rangle \\ &= E_o + \sum_{k\sigma} \left[\xi_{k\sigma} G_{\sigma\sigma}(k, \tau = 0^-) - 2\Delta_\sigma F_{\sigma\sigma}(k, \tau = 0^-) \right] \\ &- \sum_k 2\Delta F_{\downarrow\uparrow}(k, \tau = 0^-) \end{aligned} \tag{9}$$

where $E_o = -|\Delta_\uparrow|^2/g_1 - |\Delta_\downarrow|^2/g_1 - |\Delta|^2/g_o$. To find the stability of the polarized superfluid state SFP, we construct the 3x3 stability matrix out of all partial derivatives $\frac{\partial^2 E_G}{\partial \Delta_i \partial \Delta_j}$ ($\Delta_{i,j} = \Delta, \Delta_\uparrow, \Delta_\downarrow$), and check for positive definiteness of the determinant of the matrix, and of all its upper-left sub-matrices. We supplement this with analysis of the "susceptibility" $\partial P/\partial h$. Thus, for a given g_1, the stable polarized superfluid state SFP, in

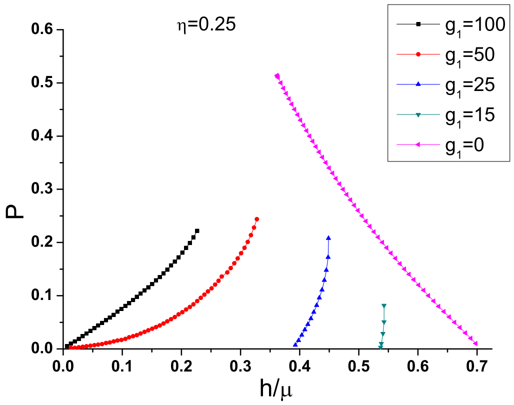

FIG. 2: (Color online) Polarization $P = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}$ vs $h/\mu = \frac{\mu_\uparrow - \mu_\downarrow}{\mu_\uparrow + \mu_\downarrow}$ (h acts like a "magnetic field") for different intra-species strengths g_1 at a fixed inter-species coupling $\eta = 0.25$.

both BCS and BEC regimes, is characterized by E_G with a *global minimum* at non-zero gaps and self-consistently determined values of μ_σ's, and $\frac{\partial P}{\partial h} > 0$. SFP sustains larger polarizations for progressively larger g_1.

Similar to the case without intra-species correlations, g_1, there exists a maximum polarization, P_{max} on the BCS side, beyond which we find no solution to the coupled equations; this determines the SFP/PS1 $\leftrightarrow$ N boundary (Fig. 1a). P_{max} is slightly decreased at unitarity by g_1. It decreases with increasing $\eta = -1/k_F a_s$. For a fixed g_1, close to both BCS and BEC sides of unitarity, and for small polarizations, unlike-spin pairing has appreciable value in the polarized superfluid SFP. However away from unitarity on the BCS side, $\Delta_{\uparrow\downarrow}$ decreases, and $\uparrow\uparrow$ and $\downarrow\downarrow$ pairing becomes more dominant in SFP, as inter-species interaction becomes relatively weak compared to intra-species interaction. On the BEC side away from unitarity, on the other hand, $\Delta_{\uparrow\downarrow}$ is more dominant, and with $\Delta_\uparrow$ and $\Delta_\downarrow$ becoming negligible, SFP becomes unstable to phase separation, PS2. A SF phase emerges deep in the BCS regime with predominantly unlike-spin pairing at low polarizations and majority spin pairing at higher polarizations.

The region PS1 in Fig 1a is characterized by *negative* "susceptibility", $\frac{\partial P}{\partial h}$ and doe not satisfy the stability matrix criteria. For a given P and h, E_G is a *maximum* at the non-zero gap solutions, separating two local minima – a feature of phase separation into a normal and a superfluid component by 1st-order phase transition. In this context, it is instructive to study P as a function of h/μ for different values of g_1, for a fixed η (shown in Fig.2 for $\eta = 0.25$ (BCS side)). For $g_1 = g_1^c \approx 15$, the slope is vertical (g_1^c is the value of g_1 at which maximum polarization, P_{max} occurs for a given η). For $g_1 \leq g_1^c$, the slope is *negative*, corresponding to the BCS superfluid state being unstable to the normal state for $h > \Delta$, but robust against polarization for $h < \Delta$. For $g_1 > g_1^c$, the singlet superfluid state can sustain a *finite polarization*, which exhibits a behavior over the range given by: $P \propto ah + bh^3 + c$; a,b,c being constants. The linear behavior is achieved for larger values of g_1, and at low polarizations. In examining P vs h/μ behavior *beyond* P_{max}, we find, for a given g_1, *two* solutions of P corresponding to one value of h/μ. To make a connection to Fig. 1a, obtained for $g_1 = 20$, we note that the allowed range of polarizations for SFP in P vs h/μ considerations corresponds to the $\eta = 0.25$ vertical line, terminating at the SFP-PS1 boundary (Fig 1a). The same line extended from SFP-PS1 boundary to PS1-N boundary correspond to the polarization range bounded by the two solutions of P at a h/μ in Fig.2. The region PS2 in BEC regime, though characterized by $\frac{\partial P}{\partial h} > 0$, is not a stable superfluid phase, since the stability matrix condition cannot be satisfied. The line separating PS1 and PS2 is probably a metastable line, the position of which depends on the p-wave interaction strength.

In summary, we find that the inclusion of intra-species correlations in asymmetrical Fermi systems results in a stable polarized superfluid phase SFP at low polarizations on both BCS and BEC sides of unitarity. We have discussed the nature of the paired states and transition to phase separated states. The SF phase obtained in the deep BEC regime in the case without intra-species correlations, also emerges here with dominant unlike-species pairing, accompanied by weaker majority-species pairing. Our results should be of broad interest as it should be of relevance to any asymmetrical Fermi system, with proper choice of interaction parameters. Here, our choice of parameters appear to agree with cold atom experiment [2] that found a SF to PS transition around $\sim 10\%$ polarization around unitarity on the BEC side. Also, the maximum polarization $\sim 70\%$ at unitarity is in agreement with experiments. Further experiments at low polarizations on both sides of unitarity are needed to test our detailed results. Experiments that measure differences in momentum distributions of two species could provide further test. Finally, our phase diagram indicates a tricritical point (SFP,PS1,N phases) at low polarization on the BCS side, in addition to one on the BEC side at $P \sim 1$. This should lead to interesting study of the evolution of these two tricritical points at finite-T; we are exploring these effects.

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